

AMENDMENTS TO THE SPECIFICATION

IN THE SPECIFICATION:

Please replace the paragraph on page 1, line 32, and bridging to page 2, line 2, with the following rewritten paragraph:

For example, when it is intended to predict the NMR chemical shift from the existing data base, stereochemical information suitable therefore has not been canonically coded. For that reason, only information on the planar structure has been used ~~in the present circumstances~~. The prediction of the chemical shift based on the data base taking account of the stereochemistry has not been realized even in any conventional chemical shift predicting computer systems.

Please replace the paragraph beginning on page 2, line 3, with the following rewritten paragraph:

In addition, there are ~~not any~~ no notation techniques capable of easily utilizing information on ~~a difference in~~ different stereostructural ~~environment~~ environments, such as conformation and configuration, between a plurality of molecules, as computer readable data.

Please replace the paragraph beginning on page 2, line 10, with the following rewritten paragraph:

It is therefore an object of the present invention to solve the above described problems of the prior art and to provide a molecular coding method for preparing ~~computer-readably~~ computer-readable and canonically ~~coding~~ coded information on the stereostructural environment, such as conformation and configuration, of a molecule.

Please replace the paragraph on page 2, line 15, and bridging to page 3, line 25, with the following rewritten paragraph:

In order to achieve the above described object, according to a first aspect of the present invention, there is provided a molecular stereochemical coding method ~~for taking a~~ wherein the stereochemistry about each of a plurality of atoms constituting a molecule ~~to code the molecule~~ is coded, the method comprising: a hierarchy classifying step of assigning a start atom, ~~which is to be noticed,~~ to a zero-th hierarchy serving as the lowest hierarchy, assigning an atom, which is ~~combined with~~ the start atom ~~on a higher hierarchy side,~~ to a first hierarchy, assigning an atom, which is ~~combined with~~ bonded to the atom assigned to the first hierarchy, to a second hierarchy, and similarly, sequentially assigning atoms to hierarchies until the ~~final~~ entire hierarchy

~~which is~~ has been set ~~so as to~~ in a form that can be specially requested by the processor; a molecular tree forming step of setting a predetermined precedence rule for placing a plurality of atoms, which belong to the same hierarchy, ~~in the~~ an order, and placing the atoms, which belong to the same hierarchy, ~~in the~~ an order ~~every hierarchy~~ in accordance with the precedence rule, to form a molecular tree ~~every the start atom from a lower hierarchy to a higher hierarchy so as to express~~ where a bonding relationship ~~between the~~ for a plurality of atoms from a lower hierarchy is described to atoms in the higher hierarchies; a coding step of noticing one of atoms, which ~~are~~ is assigned to the (n+3)-th hierarchy, with respect to each of the integers n ~~assuming that n is an integer of 0 or more~~ (assuming that n is an integer of 0 or more), in the molecular tree, deriving a dihedral angle between a plane, which is formed by an atom in the (n+3)-th hierarchy, an atom in the (n+2)-th hierarchy and an atom in the (n+1)-th hierarchy, and a plane, which is formed by the atom in the (n+2)-th hierarchy, the atom in the (n+1)-th hierarchy and an atom in the n-th hierarchy, with respect to a group comprising four atoms which consists of the noticed atom in the (n+3)-th hierarchy, the atom in the (n+2)-th hierarchy which is ~~combined with~~ bonded to the atom in the (n+3)-th hierarchy, the atom in the (n+1)-th hierarchy which is ~~combined with~~ bonded to the atom in the (n+2)-th hierarchy, and the

atom in the  $n$ -th hierarchy which is ~~combined with~~ bonded to the atom in the  $(n+1)$ -th hierarchy, replacing the derived dihedral angle into an angular symbol, which is defined in accordance with a predetermined angle dividing rule, in accordance with the magnitude of the dihedral angle, giving the replaced angular symbol to the noticed atom in the  $(n+3)$ -th hierarchy, and similarly, giving angular symbols in accordance with the magnitudes of the dihedral angles with respect to other atoms to be noticed; and setting a predetermined linear notation rule for expressing the molecular tree by a row of characters, carrying out the linear notation of a set of the plurality of angular symbols in accordance with the predetermined linear notation rule so as to correspond to the molecular tree, preparing a conformation code indicative of a conformation of the molecule with respect to the start atom, and similarly, preparing conformation codes with respect to other start atoms.